Chapter 10
Premixed Piston IC Engines

Internal combustion (IC) engines have been moving the industrial world for over three centuries. Huygens and Papin's first proposal of a gunpowder-powered engine in the 1680s started a revolution for the new industrial world. For the next 50 years, numerous types of engines (mainly steam engines) were invented and produced. Many failed to meet the commercial needs of the time, but others prevailed. An example of the first successful IC engine was Lenoir's single-cylinder, two-stroke gas engine in 1860. By the early nineteenth century, liquid fuels were made increasingly available from oil wells in the United States. The convenience of liquid fuels and their high energy density compared to gaseous fuels promoted the rise of internal combustion engines. Otto patented his first four-stroke IC engine in 1876. Otto claimed that his engine was more quiet and efficient than steam engines. Many others such as Daimler followed in Otto's footsteps. Descendants of Otto's engine, the modern spark-ignited (SI) engines can be found in every corner of the globe. Because of the high power density, low cost of production, and the vast infrastructure for gasoline, SI engines are ideal power platforms for passenger cars, small trucks, motorcycles, lawn mowers, and small electrical power generators. SI engines are robust and capable of producing high levels of power at wide speed ranges. However, SI engines usually require throttling to control the power output, which increases the engine's pumping losses and decreases overall efficiency. Current opportunities for internal combustion engine research include efficiency improvement, novel fuel implementation, and pollution reduction.

10.1 Principles of SI Engines

The premixed piston SI engine is an engine in which premixed fuel and oxidizer are introduced into the combustion chamber through an intake manifold. The combustible mixture is compressed by a piston to reach a high temperature and pressure. When the piston is near the top of the compression stroke (top dead center or TDC), combustion is initiated by a spark plug, and a premixed flame develops and propagates through the cylinder, creating gases with even higher temperature and pressure.

S. McAllister et al., *Fundamentals of Combustion Processes*, Mechanical Engineering Series, DOI 10.1007/978-1-4419-7943-8_10,

Expansion of these gases produces direct force on the piston, thereby producing useful mechanical work. Because of combustion stability problems, the spark-ignited engine requires the use of near-stoichiometric air/fuel mixtures to ensure a successful ignition event and subsequent flame propagation. As we learned in Chap. 2, a mixture (often referred to as "charge") at stoichiometric conditions produces the highest flame temperature possible and consequently the highest power output. Unfortunately, the high temperatures also generate high levels of nitric oxide (NO_x) emissions.

The thermal efficiency of a SI engine is strongly dependent on the compression ratio of the engine, thus one might attempt to improve efficiency by increasing the compression ratio. However, the amount that the compression ratio can be increased is limited by the onset of a phenomenon known as engine knock, which is the autoignition of the gases ahead of the propagating flame front in the combustion chamber. This autoignition, or knocking, is a result of compression heating of the unburned mixture by the expanding burned gases. A rapid pressure rise occurs upon autoignition of the unburned "end gas," initiating propagation of a strong pressure wave across the combustion chamber that can "scrape off" the boundary layer, exposing the piston surface to the core gas temperature. In time, piston damage may result. The high peak pressures can also damage the spark plug and head gasket. Spark-ignited engines are also notorious for cyclic variation in performance. Cyclic variation can result in loss of engine efficiency as well as increased engine emissions. Figure 10.1 shows a set of cylinder pressure traces obtained from a Pontiac 1.6 L SI engine. Note that the peak cylinder pressure varies between each cycle. The main cause of cyclic variation in SI engines is ignition lag, which is the time required for initiating a flame kernel following the passage of a spark.

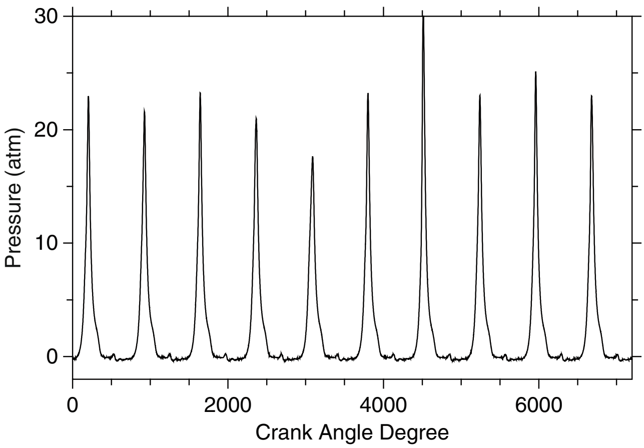

Fig. 10.1 Typical SI engine pressure traces (ten consecutive cycles)

10.2 Thermodynamic Analysis

The thermodynamic cycle that describes the SI engine is the Otto cycle. Thus, thermodynamic efficiency of a SI engine under idealized conditions (standard air assumption[1]) is given by

$$\eta = 1 - \frac{1}{CR^{\gamma-1}}, \tag{10.1}$$

where γ is the ratio of specific heats c_p/c_v, and CR is the compression ratio, V_{max}/V_{min}. It is interesting that the thermal efficiency depends only on compression ratio and γ. The temperature after the isentropic compression stroke is $T_2 = T_1 \cdot CR^{\gamma-1}$. Higher compression ratios lead to higher flame temperatures and therefore one anticipates an increase in thermodynamic efficiency. For the same reason, at a given CR, η increases with γ as shown in Table 10.1 for $CR = 8.5$.

Therefore, it is desirable to use a working media with a large γ value. The highest compression ratio that can be used in an IC engine is limited by autoignition during combustion (engine knock). The relation between the critical pressure and temperature discussed in Chap. 5 plays a vital role. As shown in Fig. 10.2 below, at the

Table 10.1 Dependence of theoretical thermal efficiency on ratio of specific heats

Working media	$\gamma = c_p/c_v$	Efficiency, η (%)
Air	1.4	57.5
CO_2	1.288	46.0
Ar	1.667	76.0
He	1.667	76.0

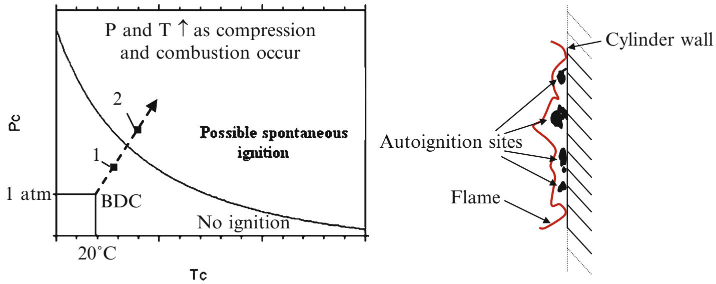

Fig. 10.2 *Left:* Autoignition can occur when critical pressure and temperature are exceeded in the engine *Right:* Engine knock occurs when unburned gases autoignite

[1] The standard air assumptions are that the mixture is entirely air that behaves as an ideal gas, all processes are internally reversible, and that the combustion and exhaust processes are heat addition/rejection processes.

beginning of the compression stroke, the mixture of fuel and air is at a temperature and pressure well below the critical pressure-temperature curve. As compression occurs, the mixture temperature and pressure increase. The mixture is typically ignited with a spark plug before the compression stroke ends (TDC). The flame then propagates through the mixture, the hot combustion products expand, and the unburned gases are further heated and compressed. Ideally, the flame will propagate through the entire mixture before the unburned gases reach the critical pressure and temperature (for instance, point 1 in Fig. 10.2). If this doesn't occur and the unburned mixture reaches state 2, autoignition can occur causing the engine to knock. Increasing the compression ratio increases both temperature and pressure at the end of the compression stroke and therefore increases the likelihood of autoignition. In addition, any hot spot in the combustion chamber can also promote autoignition.

A fuel's ability to resist knock is quantified by its octane number (for more detail, see Sect. 10.4). Increasing a fuel's octane number shifts the critical pressure-temperature curve seen in Fig. 10.2 upward, so that a higher temperature and pressure, and thus compression ratio, can be reached without autoignition. Different octane number gasolines are produced through the crude oil distillation process and by addition of chemical components. Figure 10.3 sketches power output and required octane number as function of compression ratio for a typical gasoline engine. When the compression ratio is increased, engine output increases, but a higher octane number fuel is needed to prevent autoignition. As will be discussed in Chap. 11, diesel engines operate on a different principle: autoignition of the fuel mixture is desired. In this case, the engine operates so that the temperature and pressure of the mixture at the end of the compression stroke is well above the autoignition curve, at say point 2 in Fig. 10.2.

Example 10.1 You are given a new biofuel and need to figure out if it will cause your spark ignition engine to knock. At the beginning of the compression stroke, the stoichiometric fuel/air mixture is at 25°C and 101.3 kPa. The mixture is then isentropically compressed with a volumetric compression ratio of 10. If the engine cooling system provides a convective heat transfer coefficient of 100 W/m^2−K, does the mixture autoignite? Assume that the surface area to volume ratio is 0.05 m^{-1} and the engine coolant is at 97°C. The properties of the fuel are:

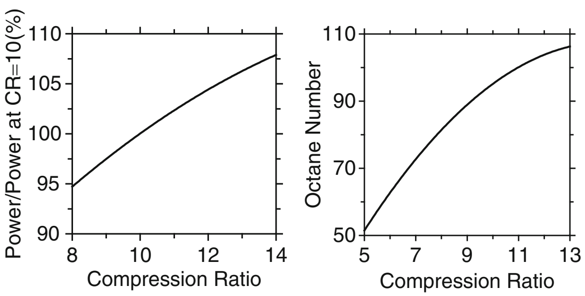

Fig. 10.3 Increasing compression ratio increases power but requires higher octane fuel

$$E_a/R = 20{,}000\text{K} \quad \hat{Q}_c{=}1.81 \text{ MJ/mol fuel} \quad a = 0.25 \quad b = 1.5$$

$$A_0 = 2.1 \cdot 10^9 \quad \text{Stoichiometric relation: Fuel} + 6.5 \cdot \text{Air} \rightarrow \text{Products}$$

Solution:
We first need to calculate the temperature and pressure of the mixture at the end of the compression stroke. Using the isentropic relations assuming the mixture is mostly air:

$$\left(\frac{T_2}{T_1}\right) = \left(\frac{V_1}{V_2}\right)^{k-1} = (10)^{1.387-1} \rightarrow T_2 = (25^oC + 273)(10)^{0.387} = 726.5\text{K}$$

$$\left(\frac{P_2}{P_1}\right) = \left(\frac{V_1}{V_2}\right)^{k} = (10)^{1.387} \rightarrow P_2 = 101.3\text{kPa} \cdot (10)^{1.387} = 2469.5\text{kPa}$$

The minimum condition for autoignition is when the heat losses balance the heat generation. Because the temperature and pressure increase during the compression stroke, the amount of heat generated by the combustible mixture will also increase so that autoignition is most likely going to occur at the end of the compression stroke. To determine whether autoignition will occur, we must evaluate the heat generated and the heat lost at the top of the compression stroke:

$$\dot{q}'''_{loss} = h\frac{A}{V}(T - T_\infty) = \left(100\frac{\text{kW}}{\text{m}^2\text{K}}\right)\left(0.05\frac{1}{\text{m}}\right)(726.5 - 370\text{K}) = 1783\frac{\text{W}}{\text{m}^3}$$

$$\dot{q}'''_{gen} = \hat{\dot{r}}\hat{Q}_c = A_0 \exp\left(\frac{-E_a}{RT}\right) x_f x_o \left(\frac{P}{RT}\right)^{a+b} \hat{Q}_c$$

$$x_f = \frac{1}{1 + 6.5 * 4.76} = 0.0313 \qquad x_o = \frac{6.5}{1 + 6.5 * 4.76} = 0.2035$$

$$\hat{\dot{r}} = \left(2.1 \cdot 10^9\right) \exp\left(\frac{-20{,}000K}{726.4K}\right)(0.0313)^{0.25}(0.2035)^{1.5} \times \left[\frac{2469.5\text{kPa} \cdot 1000\frac{\text{Pa}}{\text{kPa}}}{\left(8.314\frac{\text{Pa}\cdot\text{m}^3}{\text{mol}-\text{K}}\right)\left(100^3\frac{\text{cm}^3}{\text{m}^3}\right)726.4\text{K}}\right]^{0.25+1.5}$$

$$\hat{\dot{r}} = 1.05 \cdot 10^{-10}\frac{\text{mol}}{\text{cc} - \text{s}}$$

$$\dot{q}'''_{gen} = \left(1.05 \cdot 10^{-10}\frac{\text{mol}}{\text{cc} - \text{s}}\right)\left(100^3\frac{\text{cc}}{\text{m}^3}\right)\left(1.81 \cdot 10^6\frac{\text{J}}{\text{mol}}\right) = 191\frac{\text{W}}{\text{m}^3}$$

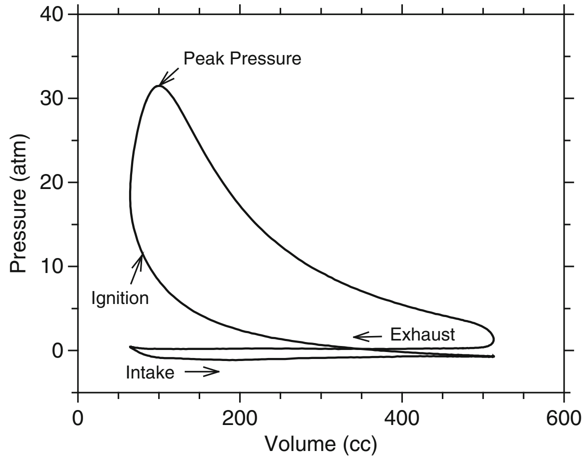

Fig. 10.4 Pressure-volume trace from a typical IC engine

Because the heat lost (1,783 W/m^3) is greater than the heat generated (191 W/m^3) the mixture will not autoignite due to the compression.

The *P*-*V* diagram of actual engines differs somewhat from the ideal Otto cycle diagram due to heat losses, friction, and the finite amount of time required for release of the fuel energy. Figure 10.4 sketches a typical pressure trace versus volume. The volume of the combustion chamber is a function of the rotational position of the crankshaft (θ), which can be measured with units of crank angle degrees (CAD) using a shaft encoder mounted on the crankshaft. With knowledge of crankshaft position and engine geometry, the engine cylinder volume can be determined by using the slider-crank formula [2].

$$V = V + \frac{\pi B^2}{4}(l + a - s) \tag{10.2}$$

where *Vc* is the clearance volume (volume at TDC), *B* is the bore (cylinder diameter), *l* is the connecting rod length (rod between crankshaft and piston), *a* is the crankshaft radius, and *s* is the distance between the center of the crankshaft and the piston and is given by

$$s = a\cos(\theta) + (l^2 - a^2\sin^2\theta)^{\frac{1}{2}}$$

The indicated work done by a piston engine between crank angle degree θ_1 and crank angle degree θ_2 can be calculated by integrating the cylinder pressure data as

$$Work = \int_{\theta_1}^{\theta_2} PdV \approx \sum_{\theta_1}^{\theta_2} P(\theta)\frac{dV}{d\theta}(\theta)\Delta\theta \tag{10.3}$$

The Indicated Mean Effective Pressure (IMEP) is defined as

$$IMEP = \frac{Work}{Swept \cdot Volume} \tag{10.4}$$

Brake mean effective pressure (BMEP) is the measured mean effective pressure from dynamometer testing of the engine. Brake specific fuel consumption (BSFC)

Table 10.2 Lower Heating Values (LHV) of some commonly used fuels

Fuel	(MJ/kmol)	(MJ/kg)
Methane (CH_4)	802.64	50.031
Propane (C_3H_8)	2043.15	46.334
Butane (C_4H_{10})	2652.34	45.73
Methanol (CH_3OH)	676.22	21.104
Iso-Octane (C_8H_{18})	5100.50	44.651

Table 10.3 Current design and operation of IC engines

IC	Operation	CR	Max. RPM	BMEP (atm)	BSFC (g/kW-h)
Small	2 S[a], 4 S[a]	6–11	4,500–7,500	4–10	350
Cars	4 S	8–10	4,500–6,500	7–10	270
Trucks	4 S	8–12	3,600–5,000	6.5–7	300
Large gas engines	2 S, 4 S	8–12	300–900	6.8–12	200
Wankel engines	4 S	9	6,000–8,000	9.5–10.5	300

[a] 2 S: 2-stroke; 4 S: 4-stroke

is a measure of an engine's efficiency. It is the rate of fuel consumption divided by power production. The indicated efficiency (η_i) is defined as followed:

$$\eta_i = \frac{Power_i}{\dot{m}_f \, LHV}, \tag{10.5}$$

where the indicated power is measured[2] in kW, $\dot{m}_f$ is the mass flow rate of fuel and LHV is the lower heating value of the fuel in MJ/kg. Table 10.2 shows the LHVs of several commonly used fuels. This definition is a thermodynamic measurement only and neglects mechanical losses such as driveline losses and oil /coolant pump losses.

Due to fluid-dynamic losses during intake and exhaust gas exchanges, the transfer of gases through combustion chamber valves is not perfect. Volumetric efficiency (η_v) is an indication of the engine's intake and exhaust performance compared to the ideal situation without any loss. Volumetric efficiency is defined as

$$\eta_v = \frac{\dot{V}_a}{V_s \cdot N}, \tag{10.6}$$

where $\dot{V}_a$ is the actual *volumetric flow rate* at standard temperature and pressure (STP) for engines without boost pressure (turbocharging or supercharging), V_s is the cylinder swept volume, and N is half the number of revolutions per second for 4-stroke engines. Since the combustible mixture is introduced into the cylinder through a relatively small opening between the intake valve and engine block, volumetric efficiency decreases with engine speed [3]. With proper tuning of an intake manifold (sometimes with the help of an acoustic box), the volumetric efficiency can be extended to higher engine speeds before it starts to decrease. Table 10.3 summarizes the typical design and operation of IC engines.

[2] When the engine is connected to a dynamometer, the power produced by an engine can be determined by $Power(\mathrm{kw}) = \frac{2\pi * Torque(NM) * RPM}{60{,}000}$.

Combustion efficiency (η_c) is a measure of how completely a mixture combusts in the engine cylinder and is defined as follows:

$$\eta_c = \frac{(\dot{m}_f\, h_f) + (\dot{m}_a\, h_a) - (\dot{m}_e\, h_e)}{(\dot{m}_f\, LHV)}, \tag{10.7}$$

where $\dot{m}_f$ is the mass flow rate of fuel into the engine, $\dot{m}_a$ is the mass flow rate of air into the engine, $\dot{m}_e$ is the mass flow rate of exhaust flowing out of the engine, and h_f, h_a, and h_e are the enthalpy of fuel, air, and exhaust gas, respectively. A combustion efficiency, η_c, of about 90% is considered as a successful combustion event. In most IC engines, about 10% of the inducted mass leaves the engine unburned due to cold boundary layers near cylinder walls and crevices.

10.3 Relationship between Pressure Trace and Heat Release

Heat release data can provide valuable information useful for better understanding engine performance. Though direct measurement of heat release rates in an engine would be difficult, heat release rate can be deduced from time histories of cylinder pressure and volume. In-cylinder pressure can be measured using a pressure transducer. Again, with knowledge of crankshaft position (CAD, θ) and engine geometry, the engine cylinder volume can be determined by using the slider-crank formula. With this information, the relation between heat release rate and pressure changes is deduced in the following:

The first law of thermodynamics gives

$$\delta Q = dE + \delta W + \delta Q_{loss} \tag{10.8}$$

The internal energy is $E = mc_vT$. For the period from compression stroke to expansion stroke, let us assume that the mass inside the cylinder is constant ($m =$ constant) and c_v is constant.

$$\delta Q = mc_v dT + PdV + \delta Q_{loss} \tag{10.9}$$

Using the ideal gas law

$$PV = mRT \tag{10.10}$$

we get $dT = d(PV)/mR$. Eq. (10.9) becomes

$$\begin{aligned} \delta Q &= \frac{c_v}{R} d(PV) + PdV + \delta Q_{loss} \\ \delta Q - \delta Q_{loss} &= \left(\frac{c_v}{R} + 1\right) PdV + \frac{c_v}{R} VdP \end{aligned} \tag{10.11}$$

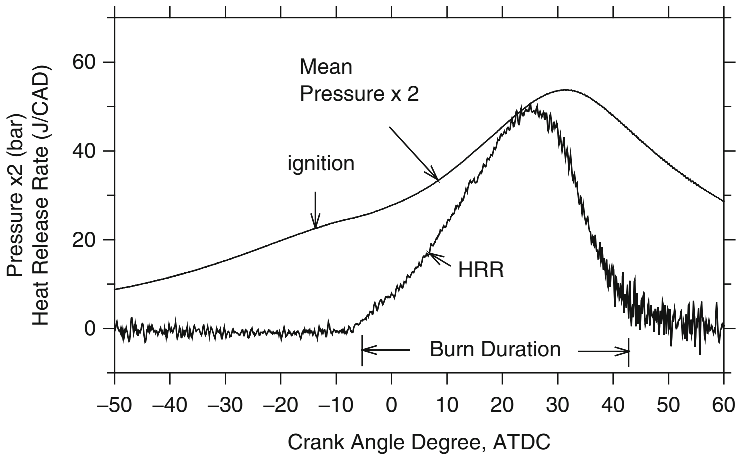

Fig. 10.5 Pressure trace and heat release rate versus CAD for a research engine with a fuel mixture of 70% isooctane and 30% n-heptane

With $c_p/c_v = \gamma$ and $c_p\text{-}c_v = R$, the net heat release rate ($\delta Q - \delta Q_{loss}$) i CAD ($\theta$) can be calculated by the following equation

$$\frac{dQ_{net}}{d\theta} = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dP}{d\theta}, \tag{10.12}$$

where $dQ_{net}/d\theta$ is the net (gross heat production minus heat losses to wall) heat release rate, γ = ratio of gas heat capacities, P = cylinder pressure, $dV/d\theta$ = the rate of change in cylinder volume with crank angle, V = cylinder volume, and $dP/d\theta$ = the rate of change in cylinder pressure with crank angle. The cylinder gas temperature can be estimated using the equation of state. Once the temperature is found, R and γ can be calculated. The rate of change of cylinder volume, $dV/d\theta$ can be calculated from the slider-crank formula. Figure 10.5 shows typical profiles of pressure and heat release rate deduced from Eq. (10.12) versus CAD for a typical engine.

10.4 Octane Number

10.4.1 Definition of Octane Rating

The octane number is a quantity for gauging the autoignition resistance of fuels used in spark-ignition internal combustion engines. The octane rating is evaluated on the basis of the knock resistance compared to a mixture of isooctane (2,2,4-Trimethylpentane) and normal heptane (n-heptane); these two fuels are referred to

as the Primary Reference Fuels (PRF). By definition, isooctane is assigned an octane rating of 100 and n-heptane is assigned an octane rating of zero. An octane number is expressed as the percentage of isooctane by volume in a mixture of isooctane and normal heptane (n-heptane) that would have the same anti-knocking capacity as the tested fuel. For example, 87-octane gasoline possesses the same anti-knock rating of a mixture of 87% (by volume) isooctane and 13% (by volume) n-heptane. However, this does not mean that the gasoline actually contains these hydrocarbons in these proportions. It simply means that the fuel has the same autoignition resistance as the described mixture of primary reference fuels. A fuel that has high tendency to autoignite is undesirable in a spark ignition engine but desirable in a diesel engine. Such a fuel would have low octane numbers. The standard for the combustion quality of diesel fuel is the cetane number to be discussed in Chap. 11.

10.4.2 Measurement Methods

The most common type of octane rating worldwide is the Research Octane Number (RON). RON is determined by running a stoichiometric fuel-air mixture through a specific variable-compression-ratio test engine, the "Co-operative Fuel Research engine" (CFR). Results obtained using the test fuel under controlled conditions are compared to results obtained for mixtures of isooctane and n-heptane. There is a second type of octane rating, called Motor Octane Number (MON) that is a better measure of how the fuel behaves when under load. MON testing uses a similar test engine to that used in RON testing, but with a preheated fuel mixture, a higher engine speed, and variable ignition timing to further stress the fuel's knock resistance. Table 10.4 lists the engine conditions of a typical CFR engine used for determining RON and MON. With mixtures of PRF containing a range of isooctane content, a reference relation between RON and compression ratio at the onset of knocking is established as shown in Fig. 10.6. The RON of a test fuel is determined by running this fuel under the same engine settings. The compression ratio at the onset of knocking is determined, say 6.75 in Fig. 10.6, and then cross-referenced to give RON = 91.6. Depending on the composition of the fuel, the MON of a modern gasoline will be about 8–10 points lower than the RON. Some example values of RON and MON are listed in Table 10.5. Normally fuel specifications require both a minimum RON and a minimum MON.

Table 10.4 Test conditions of RON and MON

	MON	RON
Engine speed (rpm)	900	600
Intake temperature (°C)	149	52
Intake pressure (bar)	1	1
Ignition time (degrees BTDC)	19–26 (Varies with compression ratio)	13

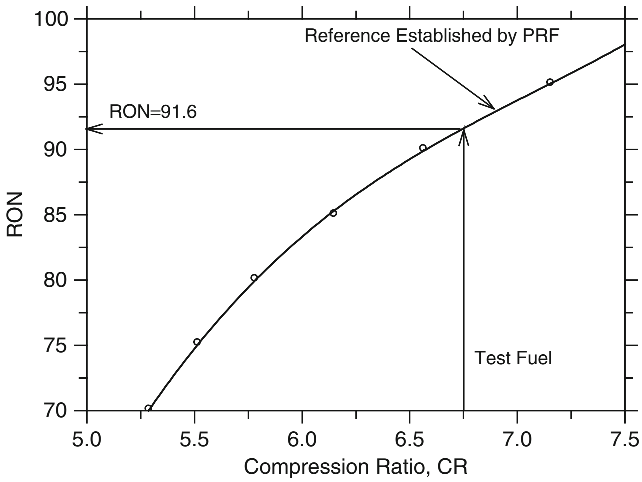

Fig. 10.6 Determination of octane number based on relation between RON and compression ratio established by mixtures of isooctane and n-heptane (PRF)

Table 10.5 Examples of octane numbers (RON and MON)

Fuel	RON	MON
n-Octane	–10	
n-Heptane	0	0
2-Methylheptane	23	
n-Hexane	25	26
2-Methylhexane	44	
1-Heptene	60	
n-Pentane	62	
1-Pentene	84	
n-Butane	91	71
Cyclohexane	97	
Isooctane	100	100
Benzene	101	
Methane	107	
Ethane	108	
Methanol	133	105
Ethanol	129	116
E85 Ethanol	105	
Toluene	114	95
Xylene	117	

In the United States, Canada, and some other countries, the headline number on the pump is the average of the RON and the MON, sometimes called the Anti-Knock Index (AKI). In many other countries, including all of Europe and Australia, the octane number on the pump is simply the RON. Because of the 8–10 point difference noted above, this means that the octane number shown on the pumps in

the United States will be about 4–5 points lower than the same fuel elsewhere. For instance, 87 octane fuel, the regular gasoline in the US and Canada, would be 91–92 in Europe.

It is possible for a fuel to have a RON greater than 100, because isooctane is not the most knock-resistant substance available. Racing fuels, straight ethanol, and Liquified Petroleum Gas (LPG) typically have octane ratings of 110 or significantly higher – ethanol's RON is 129 (MON 116, AKI 122). High octane number fuels can be used as octane booster additives.

10.5 Fuel Preparation

Premixing of fuel with air is an important step for premixed IC engines. The quality of the fuel-air mixture can greatly affect engine performance. Before the advent of electronic fuel injection, carburetors were used to mix fuel with air using a *venturi*. The top and middle of Fig. 10.7 shows how a carburetor prepares of the fuel and air mixture. The quality of fuel/air mixtures from a carburetor is not precise enough to use with three-way catalysts (see Sect. 10.9), so port fuel injection (PFI) is now widely used as sketched in the bottom of Fig. 10.7. Fuel is sprayed at the intake valve stem area when the intake valve is closed. The fuel spray usually splashes on the stem, breaking up the droplets to form a gaseous fuel-air mixture. The fuel is first pressurized by a pump to about 300 – 500 kPa, so the amount of fuel injected is controlled by the injection duration and managed by an on-board computer. However, due to the higher cost of electronic systems, carburetors are still used on small engines such as lawnmowers. The quality of fuel/air mixture can influence engine torque, with a typical relationship shown in Fig. 10.8.

Example 10.2 Estimate the power from a typical 4-cylinder 1.6 Liter 4-stroke gasoline engine at 6,000 rpm with an overall thermal efficiency of 25% and volumetric efficiency of 90%. Also determine the energy needed to vaporize the fuel and compare it to the total power produced.

Solution:
We will use isooctane as a representative fuel for cars. The stoichiometric relation is

$$C_8H_{18} + 12.5(O_2 + 3.76N_2) \rightarrow 8CO_2 + 9H_2O + 12.5 \cdot 3.76N_2$$

The power produced under standard conditions is

$$\dot{W} = \eta \cdot LHV \cdot \dot{m}_f$$
$$\dot{m}_f = \eta_v \cdot \dot{n}_{air} \cdot (FAR)_{mole} \cdot M_f$$
$$\dot{n}_{air} = \frac{V_d \cdot rpm \cdot Stroke/2}{60} \frac{1}{22.4}$$

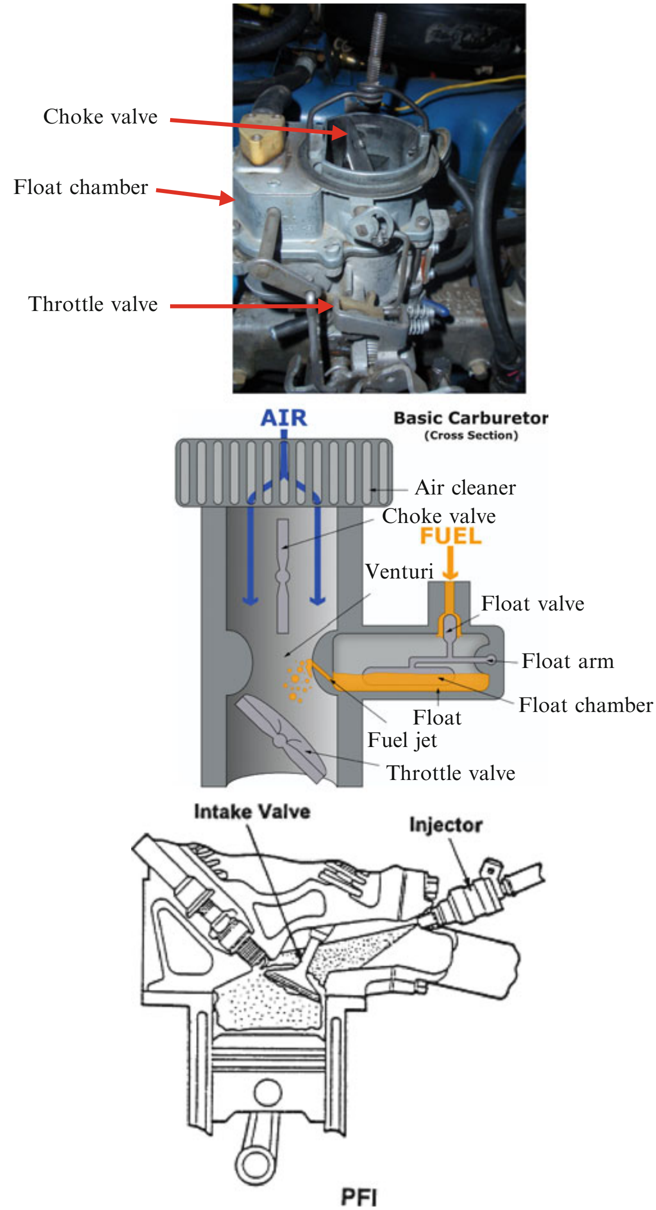

Fig. 10.7 *Top*: Carburetor and its operation within an IC engine (K. Aainsqatsi, under license CC-BY-SA-2.5). *Bottom*: Port fuel injection (Reproduced with permission from Zhao et al. [4])

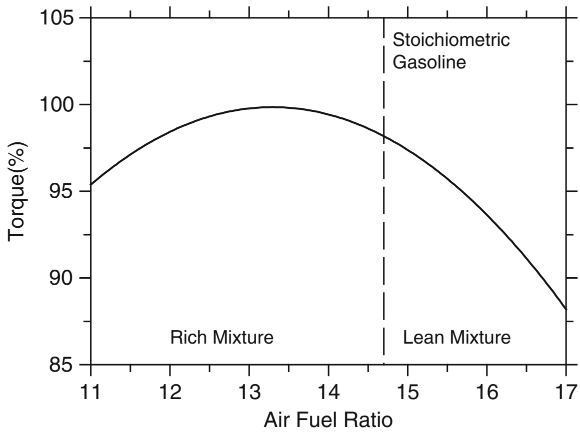

Fig. 10.8 Engine torque versus air fuel ratio (AFR)

In 4-stroke engines, every two revolutions finish one thermodynamic cycle. The total volume entering the engine is 6,000/2 × 1.6 = 4,800 Liter/min = 80 Liter/s. This corresponds to 3.57 moles of air per second that requires 0.06 moles of fuel per second (6.827 g/s) to run at stoichiometric.

$$\dot{W} = \eta \cdot LHV \cdot \dot{m}_f = 0.25 \cdot 44.65 \text{ kJ/g} \cdot 6.827 \text{ g/s} = 76 \text{ kW}(\sim 100 \text{ hp})$$

$$\text{Energy for vaporization} = h_{fg} \cdot \dot{m}_f = 283\text{J/g} \cdot 6.827\text{g/s} = 1.932\text{kW}$$

which is about 0.6% of the power produced.

Example 10.3 Consider gasoline having a chemical composition of $C_{8.26}H_{15.5}$. Determine the mole fractions of CO_2 and O_2 in the exhaust for an IC engine with normalized air/fuel ratio $\lambda = 1.2$.

Solution:
Since the overall equivalence ratio, $\phi = 1/\lambda = 1/1.2 = 0.83$, the mixture is lean. Using Eq. (2.14)

$$C_\alpha H_\beta O_\gamma + \frac{1}{\phi}\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)(O_2 + 3.76N_2)$$
$$\rightarrow \alpha CO_2 + \frac{\beta}{2}H_2O + \frac{3.76}{\phi}\left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)N_2 + \left(\alpha + \frac{\beta}{4} - \frac{\gamma}{2}\right)\left(\frac{1}{\phi} - 1\right)O_2$$

with $\alpha = 8.26$, $\beta = 15.5$, and $\gamma = 0$, we have

$$C_{8.26}H_{15.5} + \frac{12.135}{\phi}\cdot(O_2 + 3.76N_2)$$
$$\rightarrow 8.26\cdot CO_2 + 7.75\cdot H_2O + \frac{42.63}{\phi}N_2 + 12.135\cdot\left(\frac{1}{\phi} - 1\right)O_2$$

The mole fractions of CO_2 and O_2 are

$$x_{CO_2} = \frac{8.26}{8.26 + 7.75 + \frac{42.63}{\phi} + 12.135(\frac{1}{\phi} - 1)}$$
$$= \frac{8.26}{8.26 + 7.75 + 42.63\cdot\lambda + 12.135(\lambda - 1)} = 0.119$$

$$x_{O_2} = \frac{12.135(1/\phi - 1)}{8.26 + 7.75 + \frac{42.63}{\phi} + 12.135(\frac{1}{\phi} - 1)}$$
$$= \frac{12.135(\lambda - 1)}{8.26 + 7.75 + 42.63\cdot\lambda + 12.135(\lambda - 1)} = 0.035$$

Note that the dry-based mole fractions are slightly higher due to the removal of water as

$$\mathrm{dry} - based\, x_{CO_2} = \frac{8.26}{8.26 + \frac{42.63}{\phi} + 12.135(\frac{1}{\phi} - 1)}$$
$$= \frac{8.26}{8.26 + 42.63\cdot\lambda + 12.135(\lambda - 1)} = 0.134$$

$$\mathrm{dry} - \mathrm{based}\ x_{O_2} = \frac{12.135(1/\phi - 1)}{8.26 + \frac{42.63}{\phi} + 12.135(\frac{1}{\phi} - 1)}$$
$$= \frac{12.135(\lambda - 1)}{8.26 + 42.63\cdot\lambda + 12.135(\lambda - 1)} = 0.039$$

10.6 Ignition Timing

Spark ignition timing has a significant impact on the performance of an SI engine. The finite speed of turbulent flames requires that the mixture be ignited before the piston reaches top dead center in order to achieve maximum output and assure complete combustion before the exhaust valves open. Typically, ignition timing is tuned to give the best performance in terms of engine torque and pollutant emissions. To produce the maximum torque for a given rpm, the best timing is found when the peak pressure occurs around 5–10 CAD after TDC. This optimal timing is referred to as the maximum brake torque (MBT) timing as sketched in Fig. 10.9.

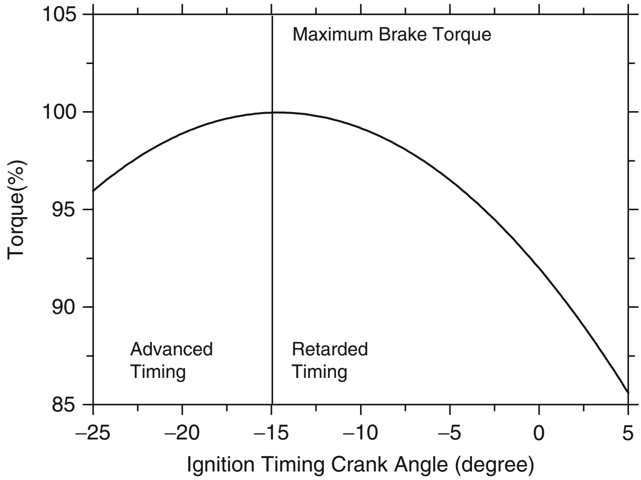

Fig. 10.9 Torque versus timing for a typical engine

Since combustion chemistry takes a certain amount of time to complete, ignition timing needs to be changed according to engine speed. When the engine speed increases, timing is advanced to achieve the best thermal efficiency. If timing is advanced too early, an engine may experience knocking. In modern engines, a knock sensor is used to detect such occurrences to protect the engine from damage. When knocking is detected, the timing of the engine is retarded slightly until knocking ceases.

10.7 Flame Propagation in SI Engines

Once the spark ignites the combustible mixture, a flame kernel develops. After a short period of time, a turbulent flame starts to form and propagate into the unburned mixture. The left picture of Fig. 10.10 was taken from the top of an optical engine showing the propagation of a turbulent flame inside a typical SI engine. Because the unburned mixture is subject to continuous compression and heating, it may autoignite, causing knocking. The pressure waves due to knock are shown on the right plot of Fig. 10.10 from a Co-operative Fuel Research Engine (CFR) for a fuel with 70% isooctane and 30% n-heptane (by volume) at CR ~ 6.0. Tremendous effort has been made to design engines that can achieve high thermodynamic efficiency by running at the highest possible compression ratios without knocking. Increasing turbulent flame speed is an effective method to increase an engine's maximum allowable compression ratio, as the residence time of the unburned mixture can be decreased, thereby reducing the chance of autoignition.

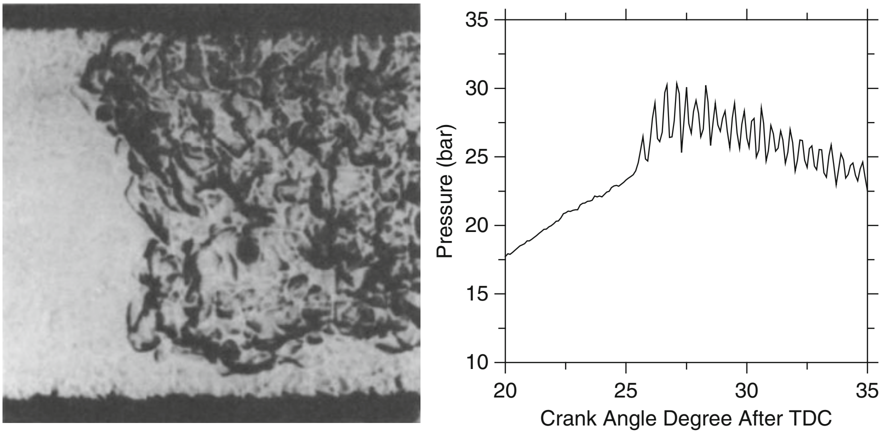

Fig. 10.10 *Left*: Picture of turbulent flame propagation inside a spark ignition engine (Reproduced with permission from Gatowski et al. [1]); *Right*: The pressure trace of an IC engine experiencing knocking shows unsteady waves

10.8 Modeling of Combustion Processes in IC Engines

Numerical models are useful tools for studying combustion processes inside an engine as well as for assisting in the design of advanced engines. Figure 10.11 presents the various physical models needed for simulation of IC engines. Due to the complexity of interactions among the different processes involved in an engine, a detailed model may demand impractically large CPU time to compute. Advancements in both Computational Fluid Dynamics (CFD) and various submodels have been made in the last two decades, and large-scale simulations using parallel computers are now run. In the foreseeable future, CFD will increase its role as an engine design tool.

The amount of CPU time required to calculate detailed chemistry can be quite severe. Figure 10.12 presents an estimate of required CPU times showing that the CPU time scales with the total number of grid cells used in CFD. In engine CFD, grid cells are used to resolve the details of the flow field, with each cell storing values of local temperature, velocity, pressure, and chemical composition. In a typical 3-D simulation, the total number of grid cells is on the order of millions. With simplified combustion chemistry, such a simulation would take a few days to a few weeks depending on the complexity of the engine geometry. Evidently from Fig. 10.12, the inclusion of detailed chemical kinetics into a detailed CFD for modeling practical engines is not practical unless a massively parallel computing facility is used. This may not be economically feasible even for a large car designer.

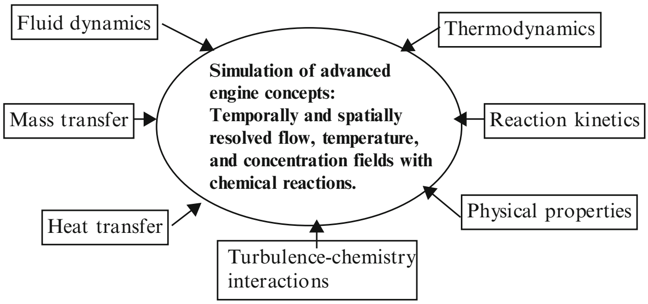

Fig. 10.11 Various physical models needed for simulations of combustion in an IC engine

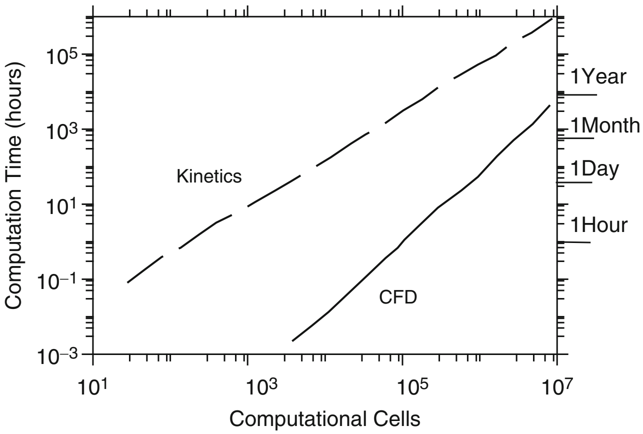

Fig. 10.12 Estimates of CPU time versus number of cells with and without combustion chemistry (From Lawrence Livermore National Laboratory)

10.8.1 A Simplified Two-Zone Model of Engine Combustion

Simplified models are often used to gain understanding of certain aspects of combustion in IC engines. The simplest model for a spark ignition (SI) engine consists of two zones, one for the burned gases and one for the unburned gases. Such a model may be used to assess overall heat release and perhaps predict the onset of knocking when an empirical model for the turbulent burning rate is properly tuned. The turbulent flame is modeled by a spherical flame front with its center located at the spark. In a more general model, the turbulent flame front can be modeled by a wrinkled front as sketched in Fig. 10.13.

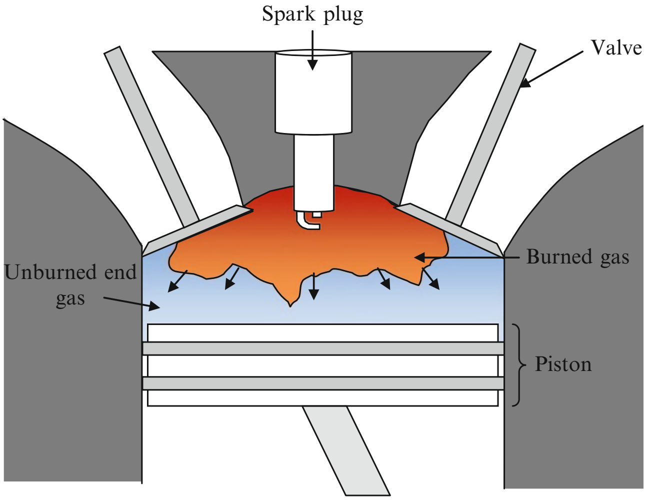

Fig. 10.13 A two-zone model for SI engine combustion with a turbulent flame front propagating from the burned zone into the unburned zoned

In most engines, experimental data indicate that the turbulent flame falls into the laminar flamelet regime[3]. Under this regime, turbulent flame speed is reasonably correlated with laminar flame speed. For engineering purposes, the turbulent propagation flame velocity is represented by an empirical model that depends on several parameters

$$\frac{S_T}{S_L} = f(u'/S_L, P/P_m, \theta_{ign}), \tag{10.13}$$

where S_T is the turbulent flame speed, S_L is the laminar flame speed, u' is the characteristic turbulent fluctuation velocity, P is cylinder pressure, P_m is the motoring pressure, θ_{ign} is the ignition timing in terms of CAD before TDC. As sketched in Fig. 10.14, the ratio S_T/S_L for general turbulent flames increases slowly with u'/S_L at low values and then increases rapidly when turbulence is intensified. For IC engines, data suggest that S_T/S_L also depends on P/P_m and ignition timing. For instance, the following empirical relation has been used in modeling engine combustion:

$$\frac{S_T}{S_L} = 1 + 1.21\frac{u'}{S_L}\left(\frac{P}{P_m}\right)^{0.82}\left(1 + 0.05 \cdot \theta_{ign}^{0.4}\right) \tag{10.14}$$

[3] Under certain regimes of turbulence-chemistry interactions, the turbulent flames consist of an ensemble of laminar flames that are merely wrinkled by turbulence. These flames are called flamelets.

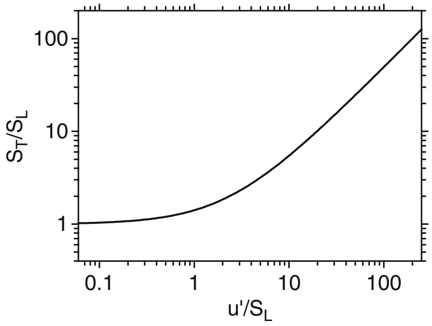

Fig. 10.14 Correlation between turbulent flame speed normalized by laminar flame speed versus turbulent fluctuation velocity normalized by laminar flame speed

The governing equations for the two-zone model include those for energy conservation, mass conservation, and two ideal gas equations:

$$\frac{d(m_u u_u)}{dt} = h_u \frac{dm_u}{dt} - P\frac{dV_u}{dt} - \dot{q}_{u,L} \tag{10.15}$$

$$\frac{d(m_b u_b)}{dt} = h_b \frac{dm_b}{dt} - P\frac{dV_b}{dt} - \dot{q}_{b,L} \tag{10.16}$$

$$\begin{aligned} m_u + m_b &= m \\ V_u + V_b &= V \end{aligned} \tag{10.17}$$

where m_u and m_b denote the masses of unburned and burned mixtures respectively, h_u and h_b are the respective enthalpies, and V_u and V_b are the corresponding volumes. Heat transfer rates to engine walls, $\dot{q}_{u,L}$ and $\dot{q}_{b,L}$, are modeled by empirical correlations. The pressure is assumed to be uniform. Using the two ideal gas equations, we have

$$P = \frac{m_u R_{un} T_u}{V_u} = \frac{m_b R_{bn} T_b}{V_b} \tag{10.18}$$

The overall mass burning rate inside an IC engine is computed by

$$\frac{dm_b}{dt} = -\rho_u \cdot A_f \cdot S_T, \tag{10.19}$$

where ρ_u and A_f are the unburned density and flame surface area respectively. One may consider the two-zone model as an extremely simplified CFD model with two grid cells. As such, detailed chemistry may be incorporated into such a simplified model. Figure 10.15 presents a typical predicted pressure trace of an IC engine running at 600 RPM using a detailed isooctane combustion mechanism

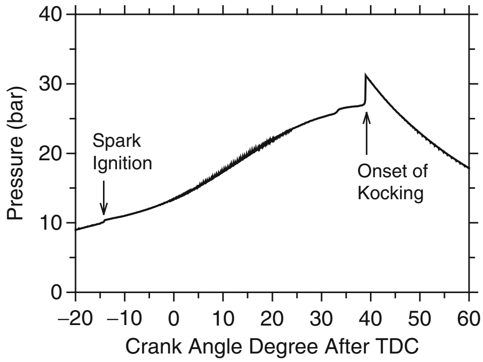

Fig. 10.15 Predicted pressure trace using a two-zone model coupled with detailed chemistry for isooctane. Ignition is initiated at 13 CAD before TDC as shown by the first pressure jump. The second pressure jump near 38 CAD after TDC indicates the onset of knocking

(856 species, 3,660 steps). Ignition is initiated at 13 CAD before TDC as shown by the first pressure jump. The compression ratio is varied to predict the onset of knocking as indicated by the small jump in the pressure trace near 38 CAD after TDC.

10.9 Emissions and Their Control

The most common emissions from a typical spark-ignition engine are summarized in Table 10.6. Most engines run with near-stoichiometric mixtures, causing high NO_x emissions in the range of 1,000 ppm. Levels of unburned hydrocarbons and CO, present primarily because of reaction quenching in the cylinder walls and crevices[4], are also high. Untreated exhaust gases can pose a severe challenge to the environment because there are so many cars on the road. The environmental impact of various exhaust species is summarized in Fig. 10.16.

Four basic methods can be used to decrease engine emissions:

1. Engineering of the combustion process
2. Optimizing the choice of the operating parameters
3. Using after-treatment devices in the exhaust system
4. Using reformulated fuels

As it was explained in Chap. 9, lean combustion is the most effective way to reduce emissions of HC, CO, and NO_x. Unfortunately, combustion instabilities in

[4] Crevices are narrow volumes present around the surface of the combustion chamber, having high surface-to-volume ratio into which flame will not propagate. They are present between the piston crown and cylinder liner, along the gasket joints between cylinder head and block, along the seats of the intake and exhaust valves, space around the plug center electrode and between spark plug threads.

Table 10.6 Typical engine emissions without treatment

HC	750 ppm[a]	CO_2	13.5 vol-%
NO_x	1,050 ppm	O_2	0.51 vol-%
CO	0.68 vol-%	H_2O	12.5 vol-%
H_2	0.23 vol-%	N_2	72.5 vol-%

[a]Based on C3

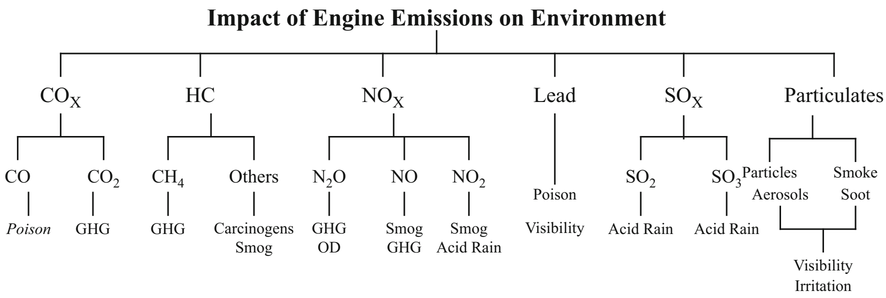

Fig. 10.16 Impact of engine emissions on the environment. GHG: Green House Gases; Ozone Depletion: OD

the cylinder limit the use of this technique in SI engines. A considerable amount of research currently attempts to improve the use of lean combustion in engines and combustors. Staged combustion – rich burning followed by lean burning – has also been used in SI engines with some success, but the accompanying reduction in power has deterred its wide implementation. Reformulated fuels, such as oxygenated gasoline in winter to reduce CO and low volatility gasoline in summer to reduce evaporative HC, are often used. Advancements in fuel injector design, oxygen sensors, on-board computers, and catalysts have lead to significant emissions reductions in SI engines in the past decades.

10.9.1 Three-Way Catalyst

Figure 10.17 gives a schematic of a three-way catalytic converter used for emission control. A three-way catalytic converter simultaneously performs three main tasks:

1. Reduction of nitrogen oxides to nitrogen and oxygen:

$$2NO_x \rightarrow xO_2 + N_2$$

2. Oxidation of carbon monoxide to carbon dioxide:

$$2CO + O_2 \rightarrow 2CO_2$$

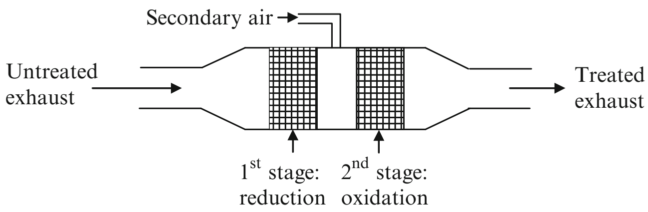

Fig. 10.17 Three-way catalytic converter with interiors exposed

3. Oxidation of unburned hydrocarbons (HC) to carbon dioxide and water:

$$2C_xH_y + (2x + y/2)O_2 \rightarrow 2xCO_2 + yH_2O$$

The catalysts used are usually a platinum/rhodium blend for the reducing reactions and a platinum/palladium blend for the oxidizing reactions. The catalytic reactions occur on the surface of the catalyst so the metals are often coated onto either a ceramic honeycomb or ceramic beads to increase the available catalyst surface area. These three reactions occur most efficiently when the catalytic converter receives exhaust from an engine running slightly lean. Typically gasoline SI engines are run with an air-to-fuel ratio between 14.8 and 14.9 (by weight), which corresponds to an equivalence ratio of 0.993–0.987. Figure 10.18 presents the transformation effectiveness of a three-way catalyst as function of product mixture. When there is more oxygen than required, the system is said to be running lean, and the system is in an oxidizing condition. In that case, the converter's two oxidizing reactions (oxidation of CO and hydrocarbons) are favored at the expense of the reducing reaction. When there is excessive fuel, the engine is running rich. The reduction of NO_x is favored at the expense of CO and HC oxidation. To compensate, additional air is often supplied to the catalytic converter in between the reducing and oxidizing stages.

In most automotive applications, an oxygen sensor (also called lambda sensor) installed in the exhaust monitors the O_2 level. The signal is used for feedback control of fuel injection duration such that the overall equivalence ratio is maintained near stoichiometric for maximum conversion of all emissions. Figure 10.19 shows the typical placement of an oxygen sensor and its voltage signal as a function of λ.

10.10 Gasoline Direct Injection (GDI) Engines

At a fixed engine speed, the amount of work produced by SI engines is controlled by a throttle plate upstream of intake manifold. When this throttling plate is partially closed, it restricts the amount of air flow, in turn restricting the amount of combustible mixture flowing into the engine. As such, for a partial load, the work required to bring combustible mixture into the cylinder increases. This loss is called

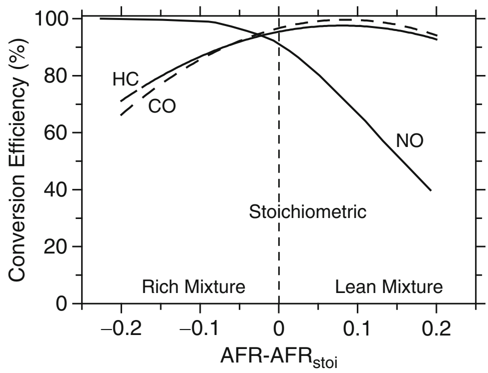

Fig. 10.18 Effectiveness of a three-way catalyst versus deviation from stoichiometric mixture

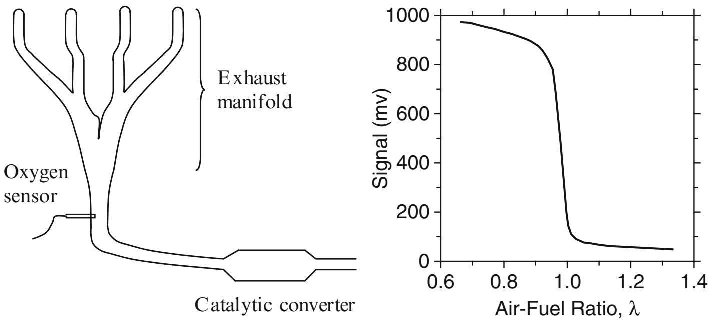

Fig. 10.19 *Left*: oxygen sensor and its typical installation in the exhaust pipe. *Right*: signal (voltage) from an oxygen sensor as function of normalized air/fuel ratio, λ

'pumping loss.' One potential means for reducing pumping loss is to manage the load by direct injection of fuel into the cylinder, similar to what is done in a diesel engine. This eliminates the need for a throttling valve and the losses associated with pulling air past the restriction. Such an engine is called a gasoline direct injection (GDI) engine and is sketched in Fig. 10.20. In principle, a throttle plate is not required in GDI engines, but in practice it is often used as a safety device. The potential benefits of GDI engines over the traditional premixed spark ignition engines with a throttling valve are: enhanced fuel economy, improved transient response, and reduced cold-start hydrocarbon emissions.

Due to the lack of a throttle plate, operating a GDI engine is more complex than a traditional gasoline engine. Figure 10.21 depicts the operation map of a typical GDI engine with three distinct modes noted. At high load (shown in the top region), a GDI engine operates similar to a traditional engine with the throttle wide open. The only difference is that fuel is injected directly into the cylinder. Injection of fuel takes place during the intake stroke of the engine to ideally generate a homogeneous mixture. To achieve a homogeneous mixture, the fuel should be injected as early as possible to allow sufficient time for vaporization of the liquid fuel as well as

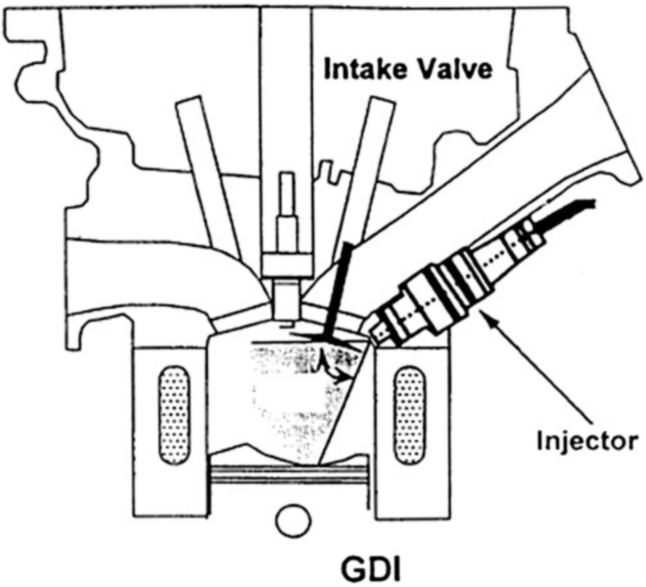

Fig. 10.20 Sketch of a gasoline direct injection engine (Reproduced with permission from Zhao et al. [4])

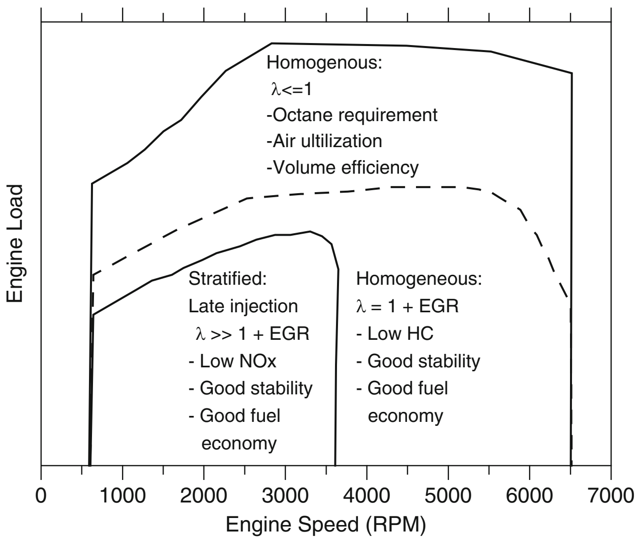

Fig. 10.21 Operation map of a typical GDI engine (Reproduced with permission from Zhao et al. [4])

subsequent mixing with air. Due to the presence of the piston near TDC, injection of fuel right after the opening of the intake valve may lead to impingement of fuel on the piston. Any wetting of interior metal surfaces inside the cylinder is undesirable, as the liquid film of fuel will not vaporize, causing large amounts of unburned hydrocarbon emission. A lean burn mode is often employed for enhancing fuel economy and lowering NO_x.

In the intermediate load regime, a homogeneous stoichiometric mixture as shown on the right is used for good running stability and fuel economy. Exhaust gas recirculation (EGR) is often used for reducing NO_x as well as for load control. Next, under the low load conditions, the amount of air taken in by the engine exceeds that required by combustion. If a homogeneous mixture is prepared by early injection, the mixture becomes too lean for flame propagation. The current method for overcoming this difficulty is to inject the fuel late in the compression stroke so that a stratified fuel-air mixture is created. Ideally, the mixture near the spark plug is near stoichiometric, making flame propagation feasible. There are two main drawbacks to such a mode: (1) In the stoichiometric region, high temperatures create high NO_x emission levels; (2) Since the mixture is stratified, a region exists where the fuel-containing mixture becomes too lean to burn; thus high levels of unburned hydrocarbons remain in the emissions. These two issues require further improvements in current GDI engines before they can be widely used in countries with strict emission laws.

Exercises

10.1 Using 87 octane gasoline, a spark-ignited internal combustion engine is designed to run at an equivalence ratio of 0.7 and a compression ratio of 9. Do you anticipate any potential problems if the engine is modified to run at a compression ratio of 12 while still running 87 octane gasoline? What about a compression ratio of 12 with 93 octane gasoline?

10.2 Assuming the spark plugs usually fire at 15 crank angle degrees before top dead center, how would the power output and emissions change if the engine was modified so that the spark plugs fire at 30 crank angle degrees before top dead center?

10.3 In a single-cylinder gasoline spark ignition premixed engine, the following data are given:

Engine geometry: bore (cylinder diameter) = 6 cm, displacement volume = 400 cm^3, compression ratio = 8
Laminar flame speed: $S_L = 70$ cm/s (constant throughout combustion)
Turbulence fluctuation: $V' = 120$ cm/s (constant throughout combustion)
Spark timing: 15 CAD BTDC ($\theta = 15$)
The following empirical formulation is used for the ratio of turbulent flame speed (S_t) to laminar flame speed (S_L)

$$\frac{S_t}{S_L} = 2 + 5 * \frac{V'}{S_L}(1 + 0.05\sqrt{\theta})$$

Estimate the total burn duration in terms of CAD at 1,000 rpm.

10.4 Considering internal combustion engines, answer the following questions.

(a) What is the purpose of an intake throttle plate commonly used in a spark ignition (SI) engine?
(b) Consider an SI engine with a volumetric efficiency of 0.85 at 2,000 rpm. How much can power be increased if the volumetric efficiency is increased to 0.95 at the same operating condition (in terms of % of power at $\eta_v = 0.85$)?
(c) The CO emissions measured in the tailpipe of a SI engine are 2,000 ppm. The calculated chemical equilibrium concentration of CO at the tailpipe conditions is 2 ppm. How is it possible that 2,000 ppm CO levels are measured in the tailpipe?
(d) What is the main purpose of a turbocharger?

10.5 In a gasoline spark ignition premixed engine running with a stoichiometric mixture, perform an analysis to determine whether or not engine knocking will occur with the following information:
Assumptions:

1. the turbulent flame propagates at a constant speed.
2. the turbulent premixed flame has a spherical shape.

Conditions, engine data, and simplifications:

1. Engine geometry: bore (cylinder diameter) = 6 cm, displacement volume = 400 cm^3, compression ratio = 8
2. Laminar flame speed: $S_L = 70$ cm/s (constant throughout combustion)
3. Turbulence fluctuation: $V' = 120$ cm/s (constant throughout combustion)
4. Spark timing: 15 CAD BTDC ($\theta = 15$)
5. Spark plug location: top center of engine cylinder
6. Unburned gas temperature = 1,650 K (constant throughout combustion)
7. Unburned gas pressure = 0.5 MPa (constant throughout combustion)

Empirical formulas:

1. The following empirical formulation is used for the ratio of turbulent flame speed (S_t) to laminar flame speed (S_L)

$$\frac{S_t}{S_L} = 2 + 5 * \frac{V'}{S_L}(1 + 0.05\sqrt{\theta[\text{CAD BTDC}]})$$

2. Empirical relation for autoignition delay of a stoichiometric gasoline-air mixture

$$\tau_{\text{ignitondelay}}[\text{ms}] = 0.08 \cdot \frac{1}{P^{1.5}[\text{MPa}]} \exp\left(\frac{3800}{T[\text{K}]}\right)$$

The units are expressed inside [ ].

10.6 From an internal combustion engine, measurements of the *exhaust* gases show that accelerating the engine speed (rpm) above a certain value increases the concentration (emission) of CO but decreases the concentration of NO. These measurements are taken right at the exhaust port before the catalyst.

(a) Explain the main reason for the emission trend *vs*. rpm.
(b) How would the emissions of pollutants change if the engine were cold or hot? Why?
(c) At a certain RPM, measurement of some (not all) exhaust species indicate: $CO_2 = 12\%$, $CO = 0.2\%$, $O_2 = 2.3\%$, and $NO = 70$ ppm. Using isooctane as the fuel, determine the NO emission index.
(d) Sketch the conversion efficiencies of an automobile catalyst for CO, HC, and NO versus equivalence ratio.

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